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13. ABSTRACT (MAX 200 WORDS):WE STUDY THE DIFFRACTION AND DECAY OF A DETONATION WAVE WHICH OCCURS WHEN ATHE DETONATION PROPAGATES PAST AN INCREASE IN CROSS-SECTIONAL AREA IN A RECTANGULAR DETONATION TUBE . IN THIS PAPER WE FOCUS ON REIGNITION BY SHOCK REFLECTION.

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NUMERICAL SIMULATION OF THE REIGNITION OF DETONATION BY REFLECTED SHOCKS

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ABSTRACT

We study the diffraction and decay of a detonation wave which occurs when the detonation propagates past an increase in cross-sectional area in a rectangular detonation tube. The computations solve the time-dependent two-dimensional *Euler equations* using an operator split Flux-Corrected Transport algorithm in an Ar diluted stoichiometric H_2/O_2 mixture. Previous studies have shown that the initial effect is the decoupling of the reaction front from the shock and the formation of a decaying blast wave or bubble in the larger tube. The detonation may then continue to decay, or be reignited by reflection of the bubble off confining surfaces. In this paper we focus on reignition by shock reflection. For a strongly overdriven initiating detonation we find that reignition occurs via an interaction between the reflected bubble shock and the original contact surface, while for more weakly driven systems reignition occurs either in the slip line and stem of the Mach reflection formed when the bubble shock reflects off the bottom surface of the tube, or by multiple shock interactions which occur at the top surface of the tube when the shocks formed by the reflected bubble overtake the initial detonation front. The computations were performed on a Cray Y-MP/216 using a fully vectorized code, and have sufficient resolution to resolve the cellular structure of the steady detonation front.

INTRODUCTION

The reignition of detonation in gas phase media by shock reflection off confining surfaces or by obstacles placed in the path of the detonation is of current interest in detonation physics. Teodorczyk et al. (1989) recently described experiments which studied the propagation of quasi-detonations. The experiments studied detonation over an obstacle and the diffraction of detonation from a corner, and the importance of shock reflections from the wall in the overall reignition process was noted. The experiments also clearly showed that if the Mach stem formed on shock reflection was strong enough then the detonation would be reignited. It appears that certain basic types of interactions involving Mach reflections or interactions between shock waves and contact surfaces or deflagration fronts are involved in the reignition of or propagation of detonations past obstacles. Simulations showing the details of some of these interactions are the subject of the present paper.

Liu et al. (1987, 1988) recently reported experiments on the transfer of detonation between gaseous explosive layers. They used a specially constructed detonation shock tube consisting of two adjacent 1.6 cm square detonation tubes three metres long ending in a test section 15 cm long which allowed the detonation ignited in one tube to diffract into the explosive mixture in the second tube. Laser schlieren photography was used to visualize the transmitted shock and detonation structures and a variety of different interaction modes were found. As the detonation reached the end of the dividing wall between the two tubes and began to expand into the test section the initial interaction consisted of the decoupling of the reaction front from the shock front and the formation of a decaying shock or bubble in the test section. The subsequent behaviour of the interaction then depended on the nature of the explosives in the two tubes. If the same explosive filled both tubes then, depending on the energetics of the particular explosive, the detonation could be reignited either directly, before the bubble reached any of the confining walls, or indirectly by reflection of the bubble off the lower wall of the tube. In the latter case detonation always appeared to occur in the region just behind the Mach stem formed when the curved bubble shock reflected off the lower wall of the tube and underwent a transition from regular to Mach reflection.

Over the last few years we have performed an extensive series of numerical simulations of the experiments of Liu et al. and have reproduced many of the interaction modes seen experimentally (Jones et al. 1990, 1991; Oran et al. 1992a, 1992b). In particular, with the same weak explosive mixture in both tubes we observed the reignition of detonation behind the Mach stem seen experimentally. These calculations had limited resolution however and the exact mechanism by which the detonation was reignited was not clearly defined. The computations were initiated using either a steady state detonation which was computed in a one-dimensional code and then introduced onto the two-dimensional grid, or by depositing an excess amount of energy into several cells of the grid, and in some cases it was found that the method of initiation influenced the final steady-state interaction pattern obtained.

To clarify these points we have performed a series of computations using a more highly resolved grid and a more controlled method of initiating the computation. Each of the runs is initiated using a detonation computed in a one-dimensional code, but the variable profiles are output at selected times well before the detonation has reached its final steady-state velocity. By this means we are able to initiate the computation using detonation profiles with specified degrees of overdrive and hence examine the effect which the strength of the initiating detonation has on both the mechanism of reignition and the final steady-state interaction pattern.

When the initiating detonation is strongly overdriven we find that detonation is reignited in the test section by the mechanism which we have previously referred to as ignition behind the Mach stem. However these more detailed calculations reveal a far more complicated mechanism. Ignition first appears at a point formed by the intersection of the reflected shock front and the original contact surface. This leads to the formation of a new shock front, and the reflection of this shock front off the lower wall of the tube gives the impression, if a low resolution grid has been used, that the ignition has occurred as the reflected bubble shock has evolved into a Mach reflection.

When a weaker detonation is used to initiate the calculation ignition no longer occurs at the intersection of the reflected bubble shock and the contact surface and the regular reflection formed on the lower surface of the test section can be observed to evolve into a Mach reflection. The reflected bubble shock then continues to move upward and is reflected again off the upper surface of the tube. This reflected shock has a higher velocity than the original decaying detonation front and eventually the two shocks collide, and it is at this point that the detonation is finally reignited. In this paper we describe these interaction mechanisms in detail, and also discuss the stability and cellular structure of the detonation front formed when the detonation is reignited by the collision mechanism which occurs on the upper surface of the detonation tube.

NUMERICAL MODEL

The simulations are based on solutions of the time-dependent Euler equations using the Flux-Corrected Transport (FCT) technique (Oran and Boris, 1987), an explicit, nonlinear finite difference technique for solving generalized continuity equations. The chemical reactions which convert gaseous reactants into detonation products were approximated using a two-step induction parameter model originally described by Oran et al. (1981) and developed further by Kailasanath et al. (1985) and Guirgius et al. (1986). The gaseous explosive consisted of a stoichiometric mixture of H_2 and O_2 diluted with Ar, the exact ratios being 2:1:7 respectively. The experimental test section was modelled using a two-dimensional rectangular Cartesian grid. Operator splitting was used in both x and y directions and the end of the splitter plate dividing the two detonation tubes was modelled by splitting the y pass into two integration loops and applying solid wall boundary conditions at the end of each loop. The grid spacing was uniform with $\delta x = \delta y = 0.04$cm (or 0.02cm for the more finely resolved calculations), and the time step was limited to 1/4 of the value given by the Courant condition, giving an average time step of 5.0×10^{-8}s (for more finely resolved calculations a time step of 2.0×10^{-8}s was used). The calculations were initiated by reading in a detonation profile from a one-dimensional version of the code.

SIMULATION RESULTS

Figure 1 shows a sequence of pressure and temperature contours for a calculation using a computational cell size of $\delta x = \delta y = 0.04$ cm and for which the initiating detonation was 24% overdriven. The degree of overdrive here is specified by the velocity of the one-dimensional detonation which is introduced onto the grid to initiate the two-dimensional detonation. In this case the detonation was travelling with a velocity 24% higher than the final steady state velocity it would have in the limit of zero overdrive.

Between t=40μs and 55μs we see that the bubble shock has formed a regular reflection on the lower wall of the tube and at t=60μs this has just transitted to a Mach reflection. The pressure contours also show some disturbance to the reflected shock front and the formation of a new shock which collides with the recently formed Mach stem at t=65μs and results in the formation of a strongly coupled reactive shock wave

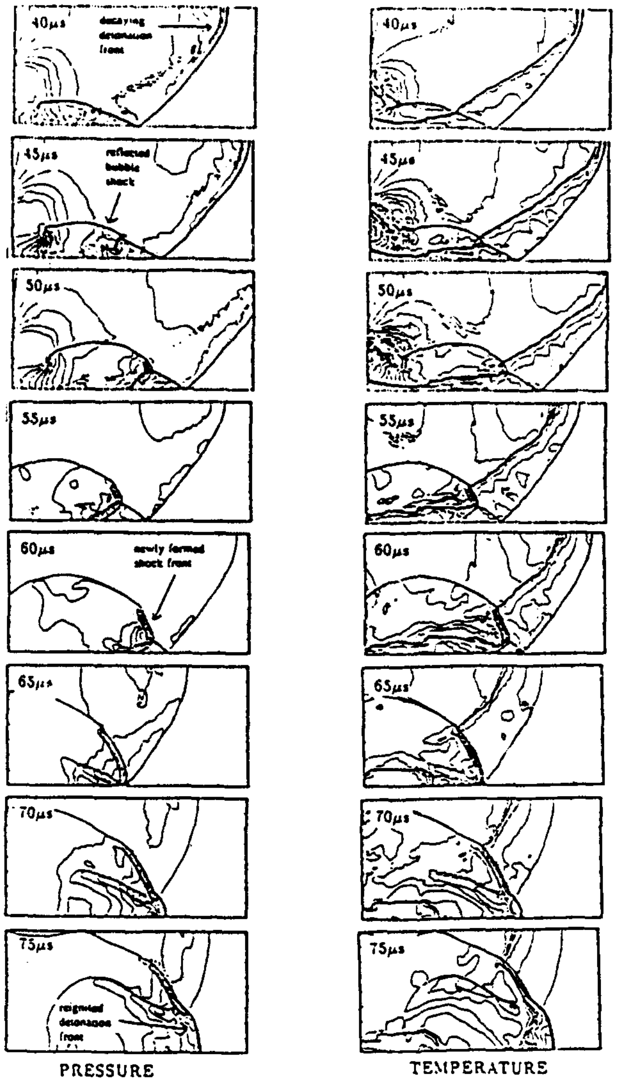

Figure 1: Pressure and temperature contours in the simulated test section for a strongly overdriven initiating detonation.

which ultimately leads to the formation of a steady detonation wave spanning the width of the test section.

The temperature contours at $t=50\mu s$ show that this disturbance is caused by an interaction between the reflected shock front and the original contact surface. The temperature contour at $t=55\mu s$ shows that the contact surface has been distorted, and that a strong reaction is occurring along that section of the contact surface which has been realigned along the direction of the reflected bubble shock. By $t=60\mu s$ the distortion of

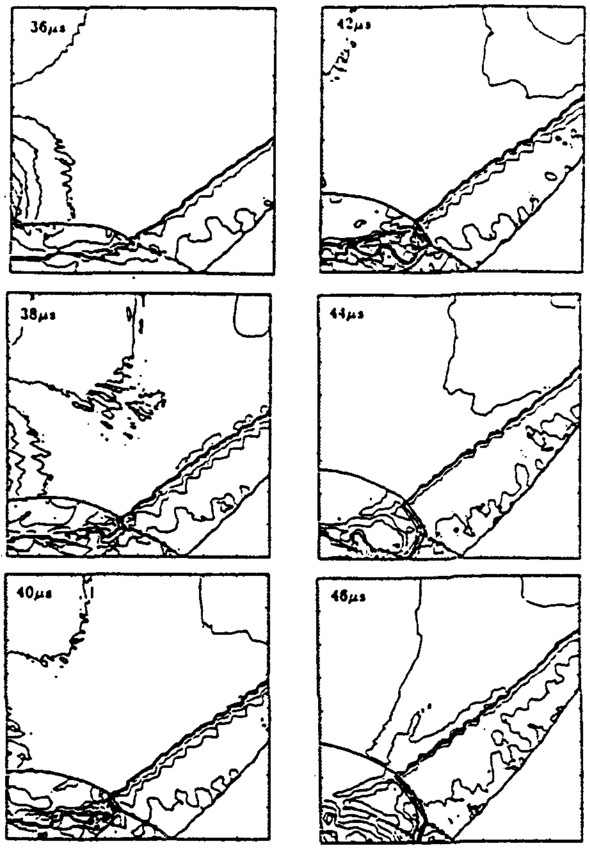

Figure 2: Simulated temperature contours in the vicinity of the ignition point for a strongly overdriven initiating detonation.

the contact surface has increased and the exothermic reaction has progressed further, and at t=65μs the reaction and associated shock front have collided with the Mach stem.

Figure 2 shows a sequence of temperature contours for a computation with a similar degree of overdrive (32%) but using a computational cell size with $\delta x = \delta y = 0.02$ cm. These more detailed contours clearly show the main features of this mode of detonation reignition. The contour at t=38μs shows that the contact surface is unstable, and the contours at t=40μs and 42μs show that these instabilities are growing rapidly. The contour at t=44μs shows that the reaction front along the contact surface appears to be increasing in intensity as the reaction is constrained by the lower wall of the test section on one side and the reflected bubble shock on the other, and the collision of this accelerating front with the newly formed Mach stem ensures that the combined structure rapidly transits to detonation.

As the strength of the initiating detonation is reduced a point is reached at which the interaction between the contact surface and the reflected shock no longer results

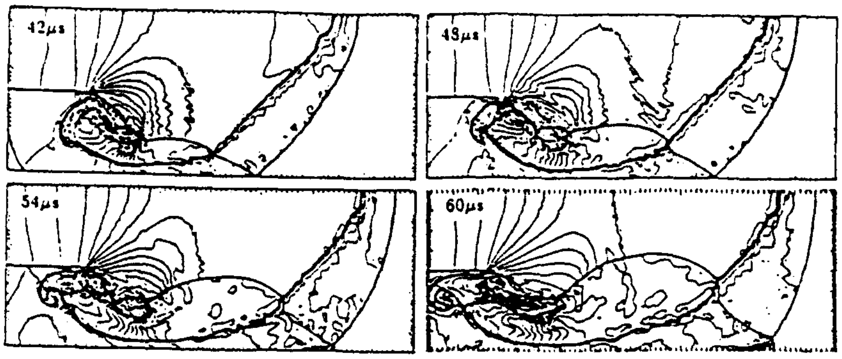

Figure 3a: Simulated temperature contours in the test section for a weakly overdriven initiating detonation.

in rapid exothermic reaction and the development of the Mach stem becomes the main feature of the flow. Figure 3 shows a sequence of pressure and temperature contours where the initiating detonation is only 1.5% overdriven, and a grid with $\delta x = \delta y = 0.02$ cm has been used. The temperature contours in Figure 3a between t=42μs and t=60μs show the reflection of the bubble shock off the lower wall and the interaction of the reflected bubble shock with the strong vortex formed at the lip of the splitter plate. At t=42μs and 48μs the reflected shock is experiencing regular reflection, while at t=54μs this has transitted to a Mach reflection. By t=60μs the Mach stem has grown, and there is evidence of reaction occurring along the slip line. Notice also in Figure 3a that there is no evidence of any exothermic reaction at the point where the reflected bubble shock intersects the contact surface, and there is no growth of the instabilities along the contact surface.

Figure 3b shows an enlarged view of the Mach stem region at times t=60μs and t=78μs. At t=60μs the temperature contours show considerable heating and reaction along the slip line and at the Mach stem, but the temperature contours at t=78μs show that this heating has been insufficient to lead to reignition of the detonation. The distance between the leading reaction front and the Mach stem has increased, and the reaction along the slip line and reaction front behind the Mach stem have failed to form the imploding detonation formation seen in the calculations of Oran et al. (1992b). This is probably due to the severe dilution of the stoichiometric H_2/O_2 mixture studied here, but may also be due to the inability of these calculations to resolve the vortex roll up along the wall.

The pressure and temperature contours in Figure 3b at t=78μs also show that the reflected bubble shock has just reflected off the upper wall of the test section. This is a regular reflection, and occurs behind the contact surface of the initiating detonation. The sequence of pressure contours in Figure 4a however show that as time progresses the reflection passes through the contact surface, undergoes a transition to a Mach reflection, and then the Mach stem catches up and collides with the leading shock front at t=108μs. Reaction variable contours (not shown here) over this same time

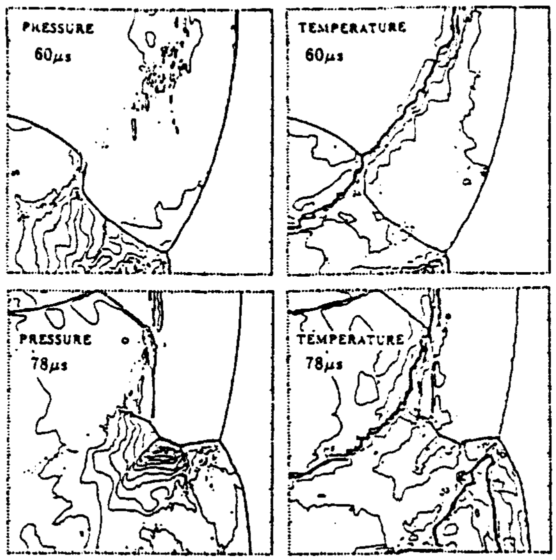

Figure 3b: Simulated pressure and temperature contours in the vicinity of the Mach stem for the detonation shown in Figure 3a.

frame show that there is no evidence of reaction occuring at the upper surface until the Mach stem of the reflected bubble shock is coincident with the weakened leading shock from the initiating detonation. At t=108μs a strong exothermic reaction starts and remains coupled to the leading shock front for the next 24μs. This is the point at which the detonation is finally reignited, and its formation is clearly evident in the pressure contours between t=114μs and t=126μs.

The subsequent behaviour of this reignited detonation is also of considerable interest. Figure 4b shows a sequence of reaction variable contours between t=132μs and t=174μs. At t=132μs a comparison between the reaction front and the shock front (visible in the pressure contours, which are unable to be included here) shows that the two fronts are still closely coupled, but at t=138μs an instability has formed and completely disrupted the detonation front. This is even more clearly seen at t=144μs. At t=150μs however the newly formed, but highly unstable, detonation front has reflected off the bottom surface of the tube and appears to have stabilised. The contours between t=150μs and t=174μs show the development of a stable detonation moving upward and into the tube, and by t=204μs (not shown) a stable detonation spanning the full width of the tube has finally been established. We have tracked this detonation for a further 40μs and the detonation continues to travel at a steady velocity, with no further sign of instability.

The nature of the detonation front in this steady-state region is also of interest.

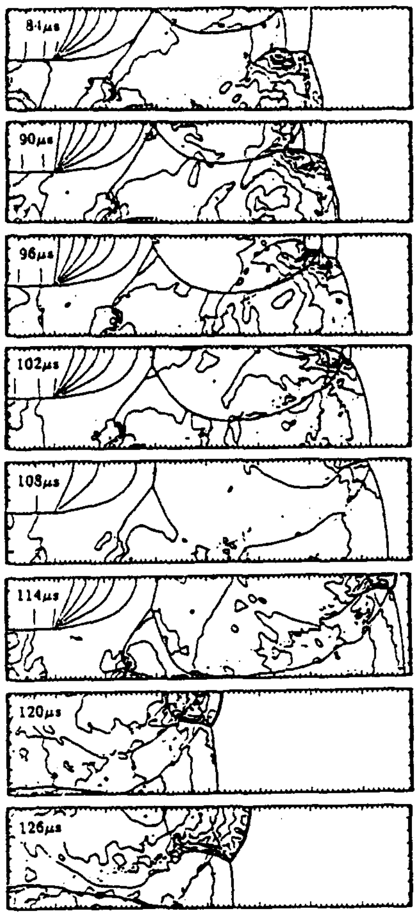

Figure 4a: Pressure contours for the detonation in Figure 3 at later times showing reignition of detonation from shock interactions at the top of the test section.

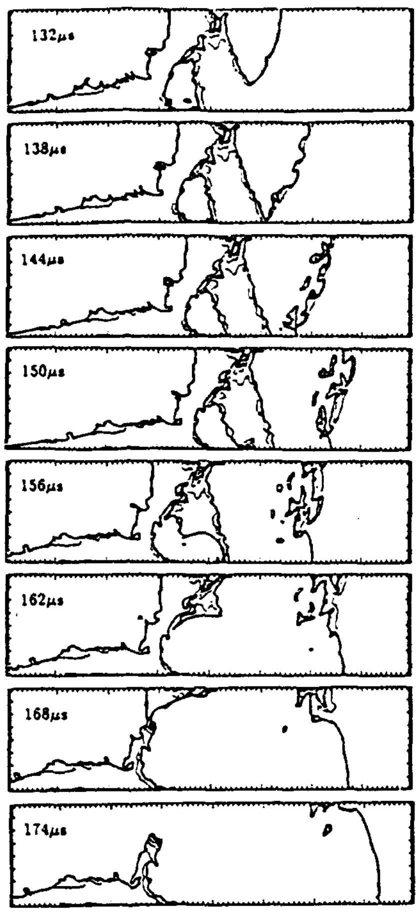

Figure 4b: Reaction variable contours for the detonation in Figure 3 at later times showing the instability of the detonation front.

Figure 5 shows pressure, temperature, density and reaction variable contours of the detonation front at $t=222\mu s$. These clearly show the cellular structure of the detonation front, which is formed by the presence of lateral shock waves moving backwards and forwards across the shock front. The points at which these transverse waves collide form a sequence of Mach stems, and it is at the triple points associated with these Mach stems that the reaction is continuously reignited, and hence the detonation sustained. As the triple points move along the tube they trace out a diamond like cellular structure which has been observed experimentally, and which can be highly regular, or irregular, depending on the nature of the explosive composition. For the highly Ar

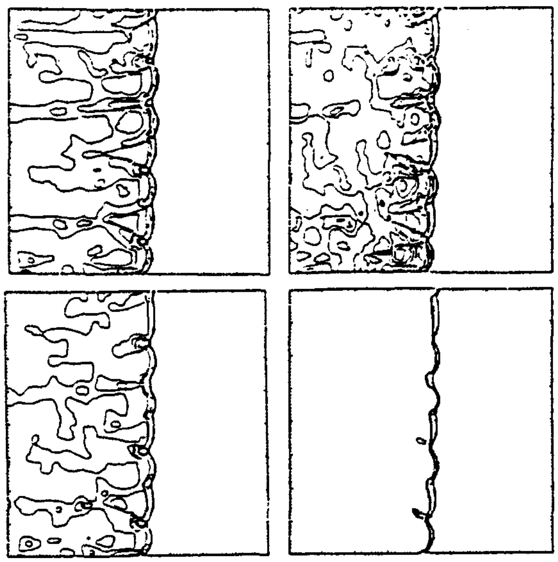

Figure 5: Pressure, temperature, density and reaction variable contours for the detonation in Figure 3 at t=222μs.

diluted stoichiometric H_2/O_2 mixture considered here, and at the initial pressure used in the simulation (one atmosphere), we would expect the structure to be irregular, and examination of the contours over successive time steps shows that this is the case. From Strehlow (1984) we can estimate that the detonation cells should have a width of approximately 0.1 cm, while our calculations indicate a size of approximately 0.45 cm. Considering the simplified chemistry model we are using in these calculations, this is quite good agreement.

DISCUSSION

The calculations presented here demonstrate several different interaction mechanisms by which a decaying detonation can be reignited. Which of these will be seen in any given situation will depend in part on the energetics of the explosive studied, and the strength of the initiating shock or detonation. If a slightly more energetic mixture had been used for these simulations, it is likely that detonation would have been reignited behind the first Mach stem formed on reflection of the blast wave off the bottom of the tube. This mechanism has been studied by Oran et al. (1992b) using a stoichiometric H_2/O_2 mixture and finer grid resolution, and the simulations clearly showed that the highest temperatures occurred from heating along the slip line and at the wall where the vortex rolled up. The temperature contours in Figure 3 also show heating along the slipline, but have insufficient resolution to resolve the vortex roll up. With more energetic mixtures and a more strongly overdriven initiating detonation, it would then be possible for reignition to occur either via the shock/contact surface interaction or along the slipline of the Mach reflection. Further simulations would be required to determine which of these would be most relevant to experimental systems of interest.

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